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Acta Materialia 51 (2003) 6181–6188



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On the proper selection of reflections for the measurement of bulk residual stresses by diffraction methods

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Received 10 February 2003; received in revised form 28 July 2003; accepted 28 July 2003

Abstract

The suitability of various reflections for diffraction measurement of bulk residual stresses in austenitic steel after plane-strain deformation is investigated by self-consistent calculations. Earlier findings (for tensile-deformed fcc materials) that 311 is particularly well suited was not confirmed. In the present calculations 111 and 422 turned out to be the best (least bad) reflections. The new results have led us to reconsider the earlier findings.

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Keywords: Micromechanical modeling; Residual stresses; Austenitic steels

1. Introduction

Residual stresses/internal stresses are of great theoretical and practical interest. Comparison between calculated and experimental intergranular stresses (type-2 stresses [1]) introduced by plastic deformation can help us to validate (or invalidate) various models for plastic deformation of polycrystals. So far most of the calculations have been based on self-consistent models, e.g. [2–7], but recently finite-element modelling has been added

[8,9]. Only measurements of *bulk* stresses are relevant in this connection. Neutron diffraction has in practice been the experimental tool of choice (e.g. [2,3,6–13]), but measurement with hard X-rays from synchrotron sources is a possible alternative, allowing stress measurements in individual grains as a supplement to the traditional measurements of average stresses in populations of grains with similar orientations [14]. The general conclusion from such comparisons is that model calculations and experiments agree quite well but not perfectly.

Residual “macroscopic” stresses (type-1 stresses [1]) have very important practical implications. They may have detrimental effects on the performance/life time of engineering components. In the present work we attempt to define the best experimental conditions for the measurement of macroscopic residual stresses. However, as to be explained, this implies the intergranular stresses

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described above. Our work thus includes the whole spectrum of theoretical and practical implications of residual/internal stresses.

When one measures macroscopic residual/internal stresses by diffraction methods (using a constant-wavelength technique), one selects one or more reflection(s) and measures the corresponding line shift(s), the lattice strain(s). Thus, one uses specific grains with specific lattice orientations as stress monitors, and these grains are not necessarily representative for the overall stress state. Normally there will be superimposed intergranular stresses. Therefore the selection of the proper reflection(s), the selection of the proper grains, is crucial. The normal rule-of-thumb is that one should select high-indices or low-symmetry reflections. In the present work we take a closer look at the suitability of various reflections—with reference to bulk stresses as measured with neutrons or hard X-rays as for instance produced in a synchrotron (in this connection measurements of surface residual stresses by traditional X-rays like CuK_α are irrelevant because they do not refer to the bulk).

The present authors [5] calculated the residual/internal intergranular stresses developed during tensile deformation of initially texture-free fcc polycrystals (aluminium, copper, austenitic steel) using Hutchinson's rate-independent self-consistent model [15]. More precisely, we calculated the lattice-strain normal components along the tensile direction and along the direction perpendicular to the tensile direction for six crystallographic planes—for six reflections—as function of the applied stress accounting for elastic anisotropy. For most crystallographic planes the lattice-strain/applied stress relation deviated very significantly from linearity. For the elastically anisotropic materials (copper and steel) the $\{311\}$ plane (the 311 reflection) came closest to linearity, i.e. the 311 reflection was most representative for the overall stress in the directions considered. For aluminium three of the six reflections—311, 331 and 531—were about equally close to linearity. For some reflections, 200 for instance, there were very great differences between the deviation from linearity for the elastically anisotropic materials copper and steel and the almost elastically isotropic

aluminium. We also monitored the slip patterns in the different materials, and we found practically identical slip patterns for the three materials apart from the very early stage of plastic deformation (the actual slip pattern was about halfway between the Taylor [16] and the Sachs [17] slip patterns). Thus, the difference in lattice strain between elastically isotropic and elastically anisotropic materials is not related to a difference in slip pattern.

Clausen et al. [10] recorded the lattice-strain/applied stress relation for an austenitic steel by neutron diffraction and found a quite good, though not perfect, agreement with the calculations in [5]. Actually the steel investigated by Clausen et al. [10] had some initial texture, and therefore they compared their measurements with calculations which were slightly different from those in [5], because the texture was included.

In the present work we repeat the calculations on austenitic steel from [5] but for plain-strain deformation in order to check the generality of the conclusion on the proper selection of reflection drawn in [5]. The present calculations include a complete mapping of the lattice strains in two-dimensional orientation space as compared to the two directions in [5].

2. The calculations

The present calculation procedure is basically identical to that in [5]. We have actually, instead of the code used in [5], used an elastic/plastic self-consistent code written by Tomé and co-workers which is basically the same as the code used by Turner and Tomé [4] on Zircaloy—because Tomé's code includes a procedure for the calculation of the lattice strains in arbitrary directions which comes in handy in the present work. The code used in [5] and Tomé's code have identical theoretical foundations, and it has been checked that they produce practically (within computational errors) identical results for identical conditions. Thus, the only real difference between the calculations in the present work and the calculations in [5] is the difference between tensile strain and plane strain, and therefore we are not going to repeat the description of the procedure. We shall

only specify the procedure for implementing plane-strain deformation. Plane strain deformation may be seen as an approximation for rolling. We therefore name the principal directions with reference to rolling: the rolling direction RD is x_1 , the transverse direction TD is x_2 , and the normal direction ND is x_3 , but the actual stresses and strains refer to plane-strain compression as executed in a channel-die compression experiment with x_1 as the non-constrained direction and x_3 as the compression direction.

During loading we enforce the following conditions:

$$\sigma_{11} = \sigma_{12} = \sigma_{23} = \sigma_{31} = 0 \quad (1)$$

$$\varepsilon_{22} = 0 \quad (2)$$

We control the deformation process by controlling ε_{33} . Since the material is texture-free and hence isotropic, it follows that

$$\varepsilon_{12} = \varepsilon_{23} = \varepsilon_{31} = 0 \quad (3)$$

and of course

$$\varepsilon_{11} = -\varepsilon_{33} \quad (4)$$

since we only consider deformation by shear. During unloading the two non-zero normal stress components are reduced to zero as shown in Fig. 1. As also shown in Fig. 1 unloading is performed at ND strains of -0.002 , -0.007 , -0.012 and -0.02 which corresponds to the unloading strains in [10]. The selection of the same unloading strains as in [10] is just an arbitrary decision with no special consequences, and therefore we have not bothered to translate the unloading strains from [10] to equivalent von Mises strains for plane strain.

In [5] we quoted the deviations from linearity as function of plastic strain for the lattice strains corresponding to the six reflections, and we stated that these deviations were practically identical to the residual lattice strains after unloading from the respective plastic strains—because there was no plastic strain during unloading. In the present work we first, for the three main directions, calculate the residual lattice strains in austenitic steel after unloading from various plane-strain plastic strains (as shown in Fig. 1) for the six reflections from [5] plus two more. By implication these residual

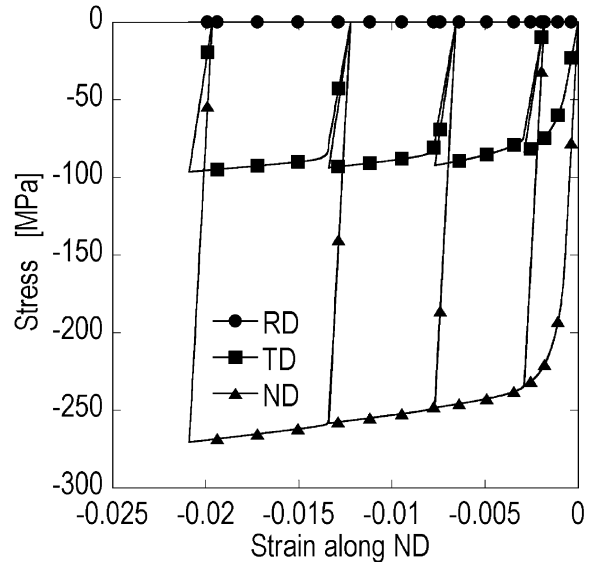


Fig. 1. The four loading/unloading sequences as illustrated by the normal stresses in the RD, TD and ND directions versus strain along ND.

lattice strains are practically identical to the deviations from linearity during loading, cf. [5]. Then we calculate the lattice strains in all directions for the eight reflections after unloading from 2% strain. The results from the latter calculations inspire supplementary calculations for tensile deformation.

3. Results

First we calculated the average residual lattice strains for the reflections 111, 200, 220, 311, 331, 420, 422 and 531 in the RD, TD and ND directions after plane-strain compression (along ND) and unloading for a “specimen” consisting of 1000 grains of initially random orientations as shown in Fig. 2. These calculations apparently confirm the results from [5], viz. that in a situation where the macroscopic residual stress is zero the 311 reflection (as indicated with broken lines) comes closest to indicate a residual stress of zero (comes closest to linearity).

However, we then decided to map out the residual lattice strains after loading to 2% plane-strain compression and unloading in two-dimen-

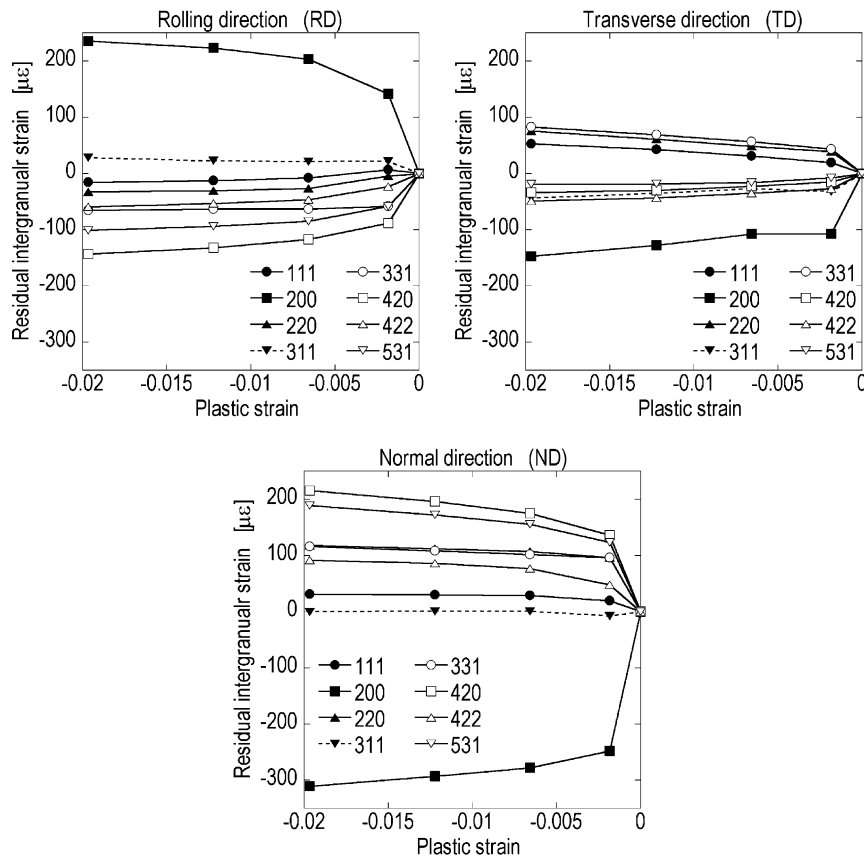


Fig. 2. Calculated lattice strains in the RD, TD and ND directions after unloading from plane-strain compression versus unloading strain along ND.

sional orientation space (in lattice-strain pole figures) for the eight reflections as shown in Fig. 3 (calculated for 10,000 grains of initially random orientations over a 2.5 by 2.5 degree grid). The largest deviations from zero for any orientation are summarized in Table 1. Now 311 does not perform particularly well. The 422 and 111 reflections have the smallest maximum deviation from zero.

4. Discussion

We have investigated the lattice strains in texture-free austenitic steel subjected to plane-strain compression and subsequent load relaxation (and by implication the derivation from linearity of the lattice strains versus applied stress) by Hutchin-

son's self-consistent model [15]. The aim is to define a "proper" selection of reflection(s) for the measurement of macroscopic residual/internal stresses by bulk diffraction methods (neutrons or hard X-rays).

In the earlier work on tensile deformation [5] (based on "measurements" parallel to and perpendicular to the tensile direction) we found that the 311 reflection was the best choice—and this conclusion was substantiated by experimental neutron investigations [10]. In the present work we find that the 311 reflection is also the best choice for measurements in the three main directions of plane strain (RD, TD and ND as referred to rolling deformation). However, we find that this conclusion does not hold for measurements in other directions. We cannot offer any explanation for the

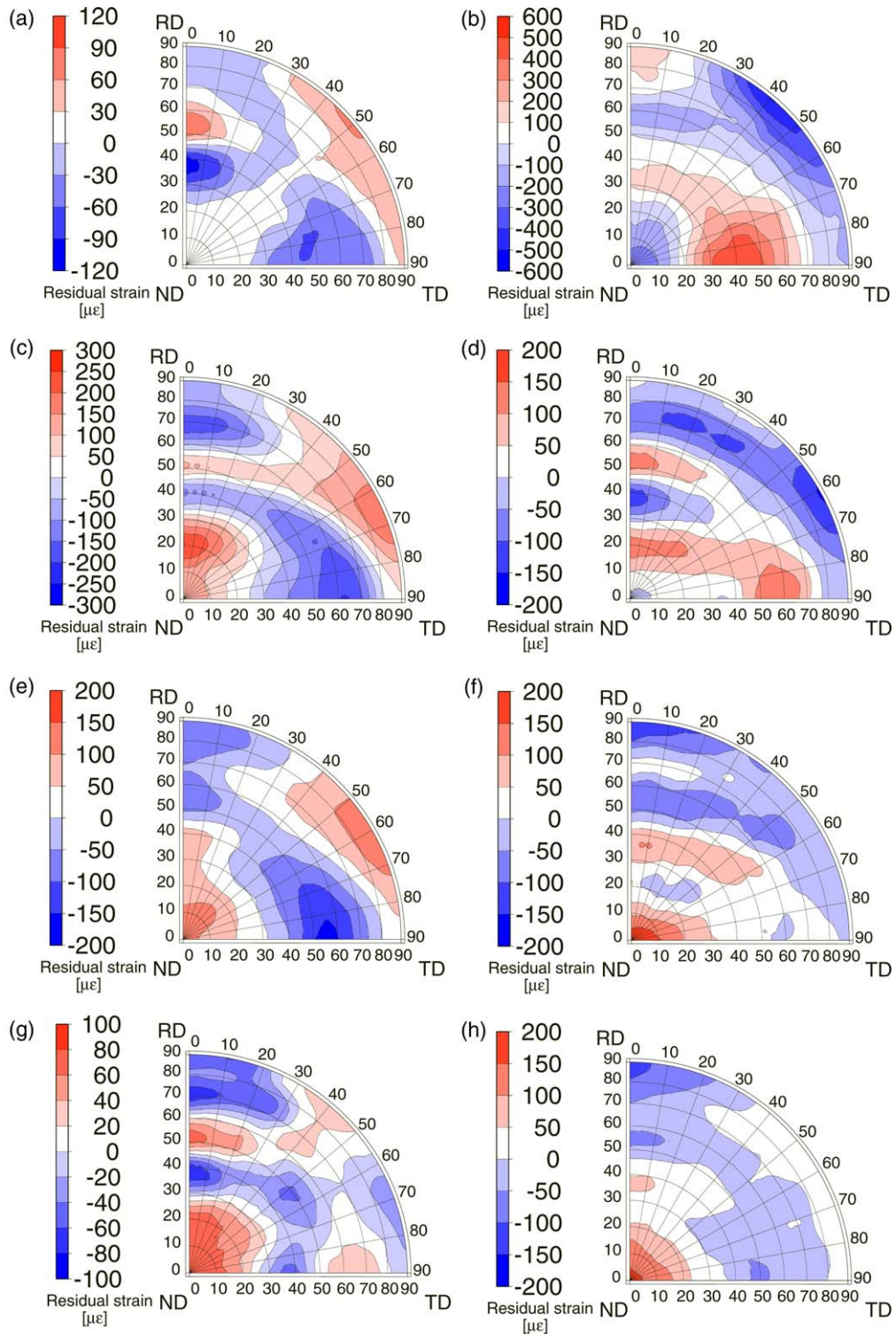


Fig. 3. Calculated residual lattice-strain pole figures for the eight reflections after unloading from 2% plane strain compression along the ND direction shown in equal-area projection.

Table 1

Calculated largest deviation from zero lattice strain (in units of microstrain) after 2% plastic strain and unloading for the eight reflections considered for plane strain and tension

Reflection	Plane strain	Tension
111	103	55
200	511	397
220	258	197
311	161	112
331	155	178
420	176	172
422	81	90
531	150	182

apparent fact that 311 is particularly well suited for measurements in the main directions both for tensile and plane-strain deformation. For our plane-strain investigation Table 1 indicates that the 422 and 111 reflections are best suited (they have the smallest maximum deviation from zero). For 111 this is quite surprising since it contradicts the generally accepted rule-of-thumb that one should go for high-indices and low-symmetry reflections. Furthermore one should notice that 111 is not just an average reflection. The $\langle 111 \rangle$ direction (perpendicular to $\{111\}$) is both elastically and plastically the hardest direction in fcc materials.

When we compare the present results for plane-strain deformation (8 reflections, all directions) with the results for tensile deformation from [5] (6 reflections, 2 directions), the obvious conclusion is that we considered too few reflections in [5] and in particular too few directions. Therefore, we have repeated the present calculations (as presented in Fig. 3 and Table 1) for tensile deformation (8 reflections, all directions) for loading to 2% strain followed by unloading. The largest deviations from zero lattice strain for any orientation are added in Table 1. Again one notices that the 311 reflection has lost its status as a particularly suited reflection and that the 422 and the 111 reflections provide the best (the least bad) indication of the macroscopic residual stress of zero. Finally one notices that the 200 reflection maintains its status as the reflection least representative for the macroscopic stress as already established in [5]. In Fig. 4 we show two examples of the residual lattice-strain pole figure

for the 422 reflection calculated for 10,000 and 1000 grains of initially random orientation deformed 2% in tension and then unloaded. For tensile deformation of an ensemble of grains of initially random orientations orientation space is ideally one-dimensional, i.e. the residual strain pole figures should have rotational symmetry. This is almost the case for 10,000 grains but not particularly for 1000 grains. Thus, we need at least 10,000 grains to get sufficiently good statistics. Close comparison of Figs. 2 and 3 shows certain inconsistencies which are explained by the relatively poor statistics in Fig. 2 with only 1000 grains. Earlier self-consistent calculations have used as low as 385 grain orientations and yielded accurate *macroscopic* results [18], but the present calculations suggest that a similar number of grains are needed within the subset of grains representing the reflections to obtain accurate results for the intergranular and residual strains.

Our preliminary conclusion, based on the results for plane-strain and tensile (and compression) deformation, is that the 111 and 422 reflections are the best indicators for the macroscopic stress state in texture-free (elastically anisotropic) fcc materials. However, with reference to our conclusion in [5] based on too few data that 311 is the best reflection, we recommend great caution when the deformation history is unknown.

Our results also indicate the magnitude of the error that may result from an “improper” selection of reflections. If we take the worst case, the 200 reflection in plane strain (Table 1), the residual lattice strain of 551 microstrain ($\times 10^{-6}$) could be converted to a residual stress of ~ 80 MPa (with the diffraction elastic constant for the 200 reflection of 150 GPa derived in [5]) instead of the correct value of zero for a specimen which has been loaded to a stress of 270 MPa and unloaded (see Fig. 1).

If we know the approximate deformation history of our specimen, we are in a much better situation to select the proper reflection(s) (and the proper measuring directions)—because we can do modelling as described in the present work. In such modelling one must include the actual texture of the specimen (in the present work we have dealt with texture-free material). If we imagine a material with a strong cube texture (with the crystallo-

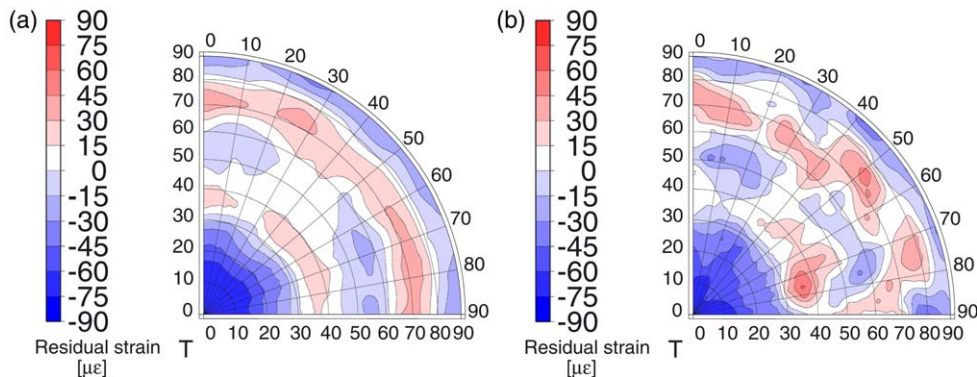


Fig. 4. Calculated residual lattice-strain pole figures for the 422 reflection after unloading from 2% tensile strain shown in equal-area projection for 10,000 grains and for 1000 grains. T stands for the tensile direction.

graphic $\langle 100 \rangle$ axes preferentially parallel to RD, TD and ND), and if we want to monitor the residual stress by measurements in the RD, TD or ND directions, we should use the 200 reflection because it represents the majority of the grains, even in spite of the fact that this is the worst reflection for texture-free material.

As to the effect of texture, we may quote the work of Pang et al. [12]. They determined experimentally the orientation distribution of the residual lattice strains in a tensile-deformed stainless steel—corresponding to our calculations in Fig. 4. Their material had a relatively weak, not rotationally symmetrical initial texture, and the resulting orientation distributions deviated very significantly from rotational symmetry. This clearly demonstrates that even weak textures have a significant effect. This may be taken as a justification for the approach in the present work, viz. to do calculations for texture-free material without having any experiments on texture-free material for comparison. As soon as actual textures are involved, parameter space soon becomes unmanageable.

Nevertheless, it is obvious that dedicated experiments with neutrons or synchrotron radiation to support (or disprove) the present results would be very important—as would all dedicated experiments to elucidate the effect of the choice of reflection(s) on the measurements of residual stresses. Considering the practical importance of residual stresses, the number of such dedicated experiments reported so far is limited. Wang et al.

[11] have measured the lattice strains in an austenitic steel rolled to 48% reduction for the reflections 111, 200, 220 and 311 in different directions in the ND/RD, the RD/TD and the ND/TD planes with neutron diffraction. 48% reduction is a much higher strain than that used in the present work, so the numerical results cannot be compared with those in the present work, but one may compare the signs of the lattice strains for the four common reflections and the common directions (those on the ND/RD and ND/TD radii and on the periphery of the pole figures in Fig. 3). It turns out that even the signs are different for many combinations of directions and reflections. However, this difference does not invalidate our calculations. The materials used in the work of Wang et al. and in our work are quite different: the material in the work of Wang et al. contains a substantial fraction (38%) of martensite and the austenite phase is strongly textured, whereas our material is a texture-free single-phase austenite. Furthermore, at the high strain dealt with by Wang et al. there is a significant contribution of mechanical twinning in the austenite phase which is a complication that we do not have to consider at the low strains in our work. One may notice that Wang et al. among the four reflections investigated find 111 to come closest to the calculated Hill results (calculations which should be basically similar to our calculations).

In the present and the earlier work we have used Hutchinson's rate-independent self-consistent model. We do not believe that the use of other advanced self-consistent models like rate-depen-

dent models would make much difference. In our opinion advanced self-consistent models (with elastic-plastic interaction between the individual grains and the continuum matrix as opposed to the elastic interaction in the first self-consistent model proposed by Kröner [19]) are among the most realistic “1-site models” [20] (models which consider individual grains interacting with a continuum matrix). It is obvious, however, that from a theoretical point of view “n-site models” [20] which consider the actual interaction of individual grains with their individual neighbour grains are more realistic than 1-site models. In practice such n-site models are normally based on finite-element modelling (FEM). However, we are not aware of any FEM results which we can relevantly compare with the present self-consistent calculations for plane strain. Dawson et al. [8] have made FEM investigations of the residual lattice strains in tensile-deformed ferritic steel. They found that the 400 reflection had a rather special behaviour in the transverse direction, which is in formal qualitative agreement with the results for 200 in elastically anisotropic materials in [5]. It is questionable whether this formal agreement (between fcc and bcc materials) is of any direct significance. But we take it as an indication that the strangest result we have seen in our self-consistent modelling, the behaviour of 200 in the transverse direction for tensile-deformed fcc materials, is not just an artefact introduced by our use of the self-consistent model in Hutchinson’s version. In connection with FEM modelling it should be mentioned that one of the present authors is involved in a synchrotron investigation of the variation in lattice strain in individual grains in tensile-deformed copper with the aim of elucidating the actual effect of the interaction between neighbouring grains (cf. [14] as cited in the introduction).

5. Conclusion

Based on self-consistent calculations (using the Hutchinson approach [15]) for plane-strain and tensile deformation of texture-free stainless steel to low strains followed by relaxation to zero macroscopic stress we find that the 422 and 111 reflections

are best suited as indicators for the macroscopic residual stress: they show the smallest maximum deviation from zero residual lattice strain for all possible measuring directions.

Acknowledgements

We thank Carlos Tomé for access to his code. B. Clausen was sponsored by National Science Foundation (CAREER grant No. 9985264). T. Leffers and T. Lorentzen acknowledge the support from the EU network TRAINSS.

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